

*What Is Claimed Is:*

1. A computer implemented method for visualizing data relating to chemical compounds, comprising the steps of:

- (1) enabling a user to select a plurality of compounds to map;
- (2) enabling the user to select a method for evaluating the similarity/dissimilarity between said selected compounds;
- (3) generating a non-linear map in accordance with said selected compounds and said selected method, said non-linear map having a point for each of said selected compounds, wherein a distance between any two points is representative of similarity/dissimilarity between corresponding compounds; and
- (4) displaying at least a portion of said non-linear map.

2. The method of claim 1, further comprising the step of:

- (5) enabling the user to interactively analyze compounds represented in said non-linear map.